Implementation of Partially Reflecting Boundary Conditions in the Generalized Maxwell-Bloch Equations

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***Abstract*—Perfectly matched layer (PML) boundary conditions have been used for several decades for the simulation of open domains within the finite difference time domain (FDTD) method. In this paper, we report on a new PML-based partially reflecting boundary condition for the generalized Maxwell-Bloch equations that enables setting a certain value of reflectance R at the end of the simulation domain. To evaluate the performance of the method, we present an error analysis and simulation results of a real optoelectronic device.**

I. Introduction

The finite difference time domain (FDTD) method is a widely applied technique for the simulation of electromagnetic fields, and has been successfully applied in the numerical treatment of the generalized Maxwell-Bloch (MB) equations [1]. For many problems, it is desirable to simulate an open domain, which led to the development of absorbing boundary conditions like, e.g., Mur's absorbing boundary conditions [2] and Berenger's perfectly matched layers (PMLs) [3]. Especially, the latter has been of great research interest in the past decades [4]. However, in all these works, the PMLs were used to truncate the simulation domain reflectionlessly. In this contribution we propose a PML-based boundary condition for the generalized MB equations that allows for setting a certain value of reflectance R at the end of the simulation window. With this, we address a recurring problem in optics, that is, a domain of interest surrounded by mirrors that partially reflect light back into the simulation domain. Alternatively, one could model partial reflections by extending the simulation domain with real materials, which could however lead to a drastic increase in simulation time. To our best knowledge, no partially reflecting boundary conditions based on PMLs have been published so far.

II. Partially Reflecting Boundary Conditions

In the following, we aim to present the implementation of partially reflecting boundary conditions into the mbsolve project, reported in [5]. The mbsolve project is an open-source software tool for the numerical simulation of the generalized, one-dimensional, full-wave MB equations. Our approach is to truncate the simulation domain with an artificial uniaxial PML (UPML) region [4]. However, instead of perfectly matching the boundary region to the simulation window, we induce a certain value of reflectance R by mismatching the relative permeability inside the PML

$$\mu_{\mathrm{PML}} = \mu_{\mathrm{r}} \left(\frac{1 \pm \sqrt{R}}{1 \mp \sqrt{R}} \right)^2 , \qquad (1)$$

where μ_{r} is the relative permeability at the end of the simulation domain. The phase of the impinging field is preserved for a positive sign in the numerator of (1). A negative sign in the numerator leads to a phase-change of π. As the negative case would lead to very small permeabilities, and thus stability issues, we restrict ourselves to the phase-preserving case. Reflections are solely introduced by μ_{PML}, while the quantum system within the MB framework is extended into the PML.

III. Error Analysis

To evaluate the performance of our method, an error analysis has been conducted, where a Gaussian pulse was injected at the left side of a vacuum simulation region. Here, no quantum mechanical system has been considered. The pulse had a center frequency of 500 THz and a FWHM bandwidth

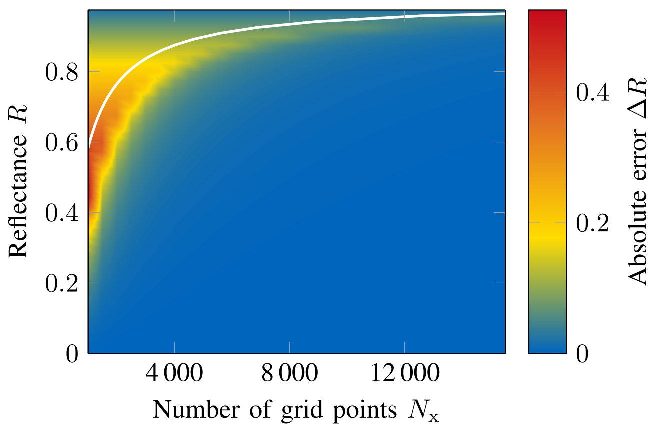

Figure 1. Absolute error for different numbers of grid points and reflectance values. The white line depicts the Nyquist limit.

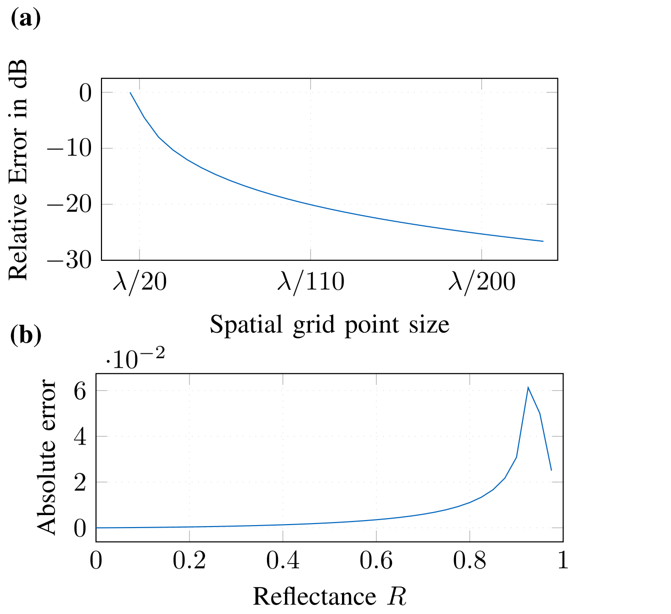

Figure 2. (a) Relative error for different spatial discretizations for a reflectance of $R = 0.5$. (b) Absolute error for different reflectance values and $N_{\mathrm{x}} = 11000$ grid points.

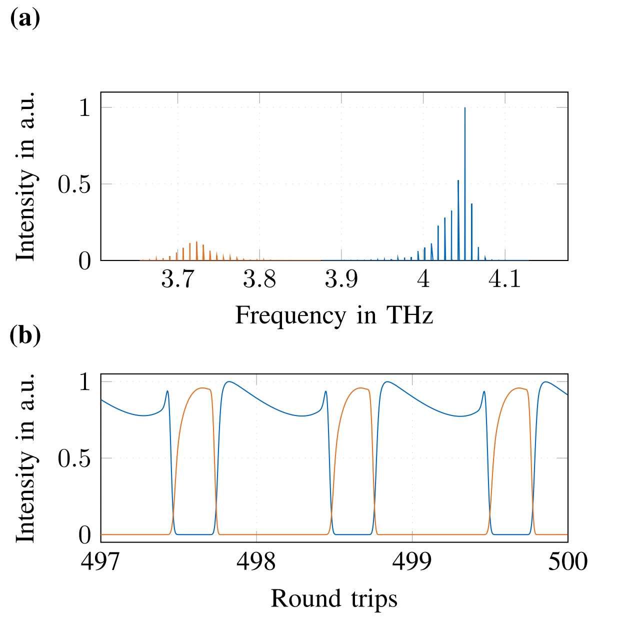

Figure 3. (a) Intensity spectrum of the QCL frequency comb from [6] at the facet of the device. (b) Envelope of the electric field for three round trips. In both plots the higher frequency components are displayed in blue, while the lower frequency components are shown in orange.

of 21 %. At the right side of the region a reflectance R has been set with the implemented partially reflecting boundary conditions. From the fields scattered back into the simulation domain, the reflectance R, was calculated as the inverse ratio of the field energies before and after reflection. With a center frequency of 500 THz the $\lambda/20$ and $\lambda/200$ limits would lie at approximately 1 300 and 13 000 grid points. Figure 1 shows the absolute reflection error for a varying number of grid points in the simulation domain and different reflectances R. The simulation results for a reflectance of $R = 0.5$ can be seen in Fig. 2 (a). In Fig. 2 (b) we show the absolute error, where the reflectance has been changed from 0 to 0.975 for 11 000 grid points in the simulation domain.

IV. Results and Discussion

From the error analysis we can identify two trends. First, the error increases for bigger values of R. Second, a decrease of the error is observable if more grid points N_{x} in the simulation domain are chosen. The reason for this is likely the discretization error associated with a prefactor in the temporal FDTD update equations, which assumes a very small value due to an increasing μ_{PML} for large R. Furthermore, the maximum absolute error in Fig. 1 and Fig. 2(b) can be explained by the fact that for a small number of grid points the Nyquist sampling theorem is violated which leads to a virtually decreased error due to artificial aliasing. The Nyquist limit is plotted as white line in Fig. 1.

The partially reflecting boundary conditions are tested on a well-studied quantum cascade laser (QCL) frequency comb, reported in [6]. Full-wave simulations of the device, were already published in [7]. With our boundary conditions we were able to reproduce the experimental and simulation data from the literature, as depicted in Fig. 3.

V. Conclusion

In this paper, we presented a PML-based boundary condition that allows to set a certain value of reflectance R at the end of the simulation domain. By conducting an error analysis we could validate our approach and evaluate the performance of our method. We saw that the accuracy of the method decreases for larger reflectances or less grid points. By simulating a QCL frequency comb as an example of a real optoelectronic device, we presented a first application of our method.

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